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PHENOMENOLOGICAL MODELING OF INFRARED SOURCES: RECENT ADVANCES

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ABSTRACT Infrared observations from planned space facilities (e.g., ISO, SIRTf) will yield a large and uniform sample of high-quality data from both photometric and spectroscopic measurements. To maximize the scientific returns of these space missions, complementary theoretical studies must be undertaken to interpret these observations. A crucial step in such studies is the construction of phenomenological models in which we parameterize the observed radiation characteristics in terms of the physical source properties. In the last decade, models with increasing degree of physical realism (in terms of grain properties, physical processes, and source geometry) have been constructed for infrared sources. Here we review current capabilities available in the phenomenological modeling of infrared sources and discuss briefly directions for future research in this area.

1. INTRODUCTION & OVERVIEW

Infrared radiation is the primary tracer of the dust component in the universe. Dust grains, although a minor constituent, play a very important role in the thermodynamics and evolution of many astronomical objects. In the last decade, NASA has launched a number of space-based observatories: the Infrared Astronomical Satellite (IRAS), the Hubble Space Telescope (HST), and the Cosmic Background Explorer (COBE). The IRAS, launched in 1983, carried out a comprehensive infrared survey of the sky and a wide variety of astronomical objects were detected in the infrared. The IRAS has stimulated advances in most branches of astrophysics and the IRAS database remains a vital tool for current research in infrared astronomy. Most recently the astronomical community in the US has identified the 1990's as the decade of infrared astronomy.

To maximize the scientific returns of past and future space missions (e.g., ISO and SIRTf) complementary theoretical studies have been undertaken. A vital component of these studies is the construction of phenomenological models in which we seek to parameterize the observed radiation characteristics of infrared sources in terms of their physical source properties (see Figure 1).

Scoville and Kwan 1976; Rowan-Robinson 1980; Wolfire and Cassinelli 1986, Egan et al. 1988). In the last decade, significant progress has been made in the development of radiation transport models for infrared sources. Models with increasing degree of physical realism have been constructed. In Figure 2 we summarize schematically the recent advances made. Clearly models of infrared sources have become increasingly sophisticated. Below we briefly describe a few selected results to demonstrate the recent progress made in the modeling of infrared sources.

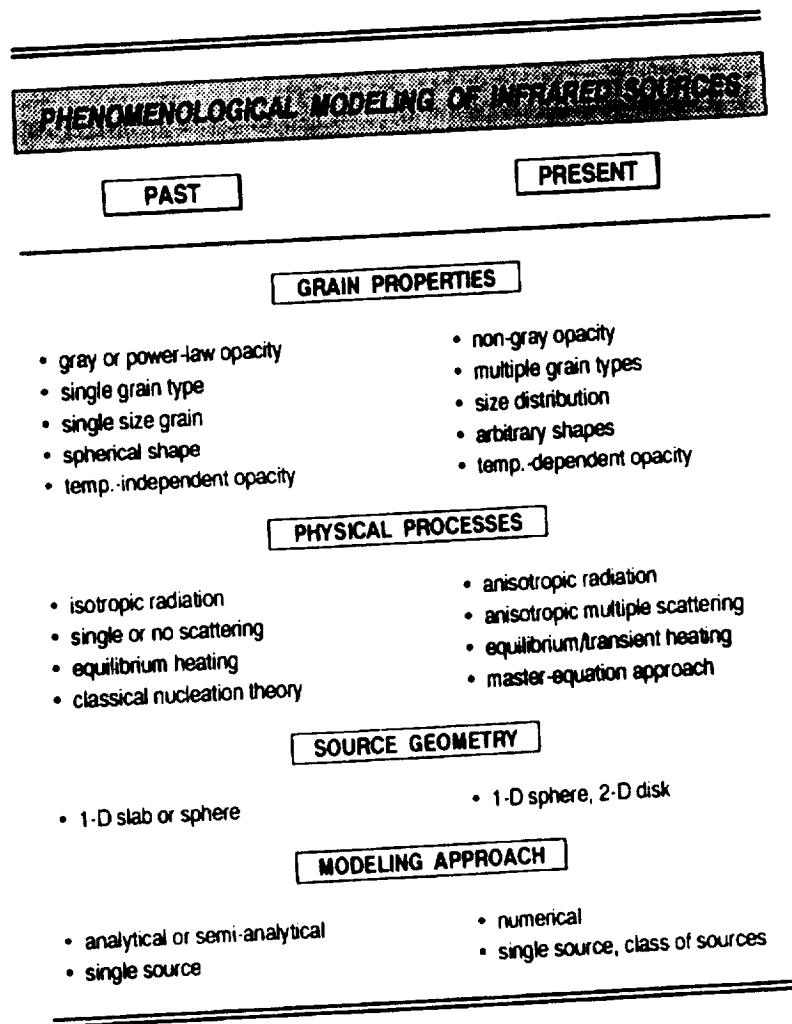


Figure 2 - Schematic diagram comparing the past and present capabilities in the phenomenological modeling of infrared sources.

THEORETICAL STUDIES OF INFRARED SOURCES

1. Perform *statistical analyses and correlation studies*, and develop *classification schemes*, e.g., histograms, two-color diagrams, correlation plots, classification of spectral features.
2. Construct *phenomenological models* for each class of objects to parameterize the observed radiation characteristics in terms of their physical source properties.
3. From the phenomenological models, develop *self-consistent physical models* which can explain coherently present and future observations.

CONSTRUCTION OF PHENOMENOLOGICAL MODELS

INPUT

- luminosity and spectral energy distribution of heat source
- source geometry & dimensions
- properties of grain species (e.g., opacity, albedo, scattering phase function)
- density distribution of dust grains
- other local heating mechanisms (e.g., viscosity, collisions with gas particles)

OUTPUT

- temperature distributions of each grain species
- characteristics of internal radiation field
- intensity variation across source surface at different wavelengths
- characteristics of grain spectral features
- emergent energy spectrum of heat source and dust shell

OBSERVATIONAL CONSTRAINTS & DIAGNOSTIC PROBES

- spectral energy distribution (flux spectrum) \Leftrightarrow source luminosity
- surface brightness & apparent emission size as a function of wavelength \Leftrightarrow dust density distribution & geometrical source size
- strength and shape of emission/absorption features \Leftrightarrow grain composition & source opacity
- color temperatures in different parts of spectrum \Leftrightarrow dust temperature distribution
- flux ratios or color-color diagrams \Leftrightarrow source evolution

Figure 1 - Schematic diagram to show that a crucial step in the theoretical studies of infrared sources is the construction of phenomenological models.

To model the observed characteristics of an infrared source, typically one solves the equation of radiation transport in a dusty medium, subject to the constraint of radiative equilibrium. For spherically symmetric geometry, the problem has been solved by many authors (e.g., Leung 1975; Apruzese 1976; Jones and Merrill 1976;

2. SOME RECENT ADVANCES

2.1 Grain Properties

In astrophysical environments dust grains have irregular shapes most likely formed by fractal growth processes, e.g., particle-by-particle aggregation or cluster-by-cluster aggregation (Witten and Cates 1986). On the other hand, spherical dust grains are often assumed in models of infrared sources so that the dust opacity can be calculated from the Mie theory. A computational technique now exists for calculating the dust opacity for grains of irregular shapes (Draine 1988; Bazell and Dwek 1990). In this method, called "discrete dipole approximation", a fractal grain is approximated by a collection of dipoles. Using realistic dust opacities for fractal grains, recently Fogel and Leung (1992) have constructed radiation transport models for infrared sources. Compared to models with spherical grains of the same composition and volume, models with fractal grains show a shift in the peak flux toward longer wavelengths, implying that *fractal dust grains are cooler than spherical grains*. These differences can be attributed to a lower ratio (p) of volume to geometric cross section (averaged over orientation) for the less compact fractal grains. The ratio p varies with the fractal dimension. Grains with a higher p attain a higher temperature. Furthermore, *grains having the same fractal dimension show almost no difference in their absorption cross sections and energy spectrum, implying that the overall grain shape plays only a minor role in the thermal properties*.

In modeling infrared sources, the opacity of dust grains is often assumed to be temperature-independent. However, the optical constants of many grain types actually change with grain temperature. In particular, for water ice, which has a feature at 3.1 μm , the absorption coefficients change with temperature. The ice feature is seen in the spectra of molecular clouds and circumstellar dust shells of both young and evolved stars (Whittet 1992). As the temperature increases, water ice changes from an amorphous state to a crystalline state. This irreversible phase change, which occurs at around 100 K, narrows the ice feature and increases the peak strength, thus producing different profiles for the 3.1 μm feature as the temperature increases. Since the grain temperature changes with position in infrared sources, it is crucial that temperature-dependent effects in grain opacity be incorporated in detailed models to interpret observations of ice features. This will allow us to probe the evolution of ice mantle on grains. Recently laboratory data on temperature-dependent optical constants for water ice (Hudgins et al. 1992) have become available, making it possible to include these effects in radiation transport models. Work is underway to study this problem.

2.2 Physical Processes

Among the unexpected results from IRAS was the discovery of excess mid-infrared emission detected in many infrared sources, e.g., diffuse clouds, dark globules, visual reflection nebulae, and high-latitude dust clouds or infrared cirrus. It is now believed that the emission at short wavelengths ($< 30 \mu\text{m}$) comes from transient heating of very small grains and large polycyclic aromatic hydrocarbons or PAHs (for a review see

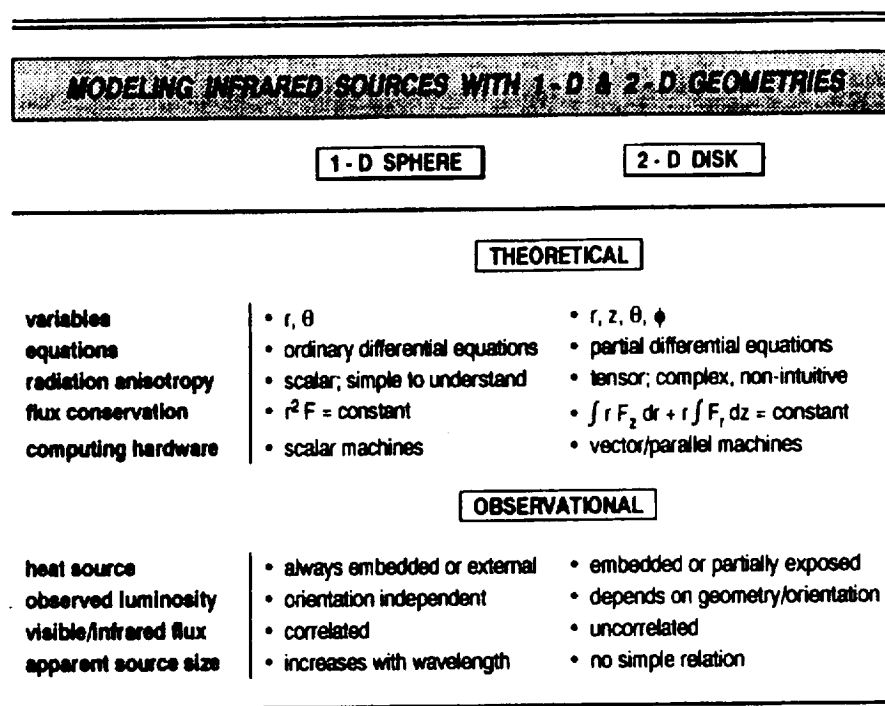


Figure 3 - Schematic diagram comparing the theoretical and observational considerations in modeling infrared sources with 1-D and 2-D geometries.

2.4 Modeling Approach

Unlike ground-based observations, space missions generally yield large quantities of data. Interpreting such data requires a different strategy which utilizes extensive modeling. As an example, the IRAS survey has yielded a large and uniform sample of high-quality data from observations of asymptotic giant branch stars. In particular, the IRAS data indicates that many carbon stars, especially those with optically thin dust shells, have large fluxes at 60 and 100 μm . It has been suggested that either an extended single dust shell or a two-shell model, with a remnant shell from an earlier mass-loss episode (Willems 1987), can explain the excess fluxes. To test these hypotheses, models of dust around carbon stars have been constructed: models with either a single C-rich dust shell or double shells (Egan and Leung 1991). Figure 4 shows the color-color diagrams for selected carbon stars in the IRAS-LRS catalog. The thick solid line is the blackbody line. The gray-shaded areas indicate the limits on the colors for carbon stars of various ages imposed by the models. Clearly single-shell models cannot explain the observed color distribution, while two-shell models with

Puget and Leger 1989). Temperature fluctuations in small grains occur whenever the energy input from photons or energetic particles is considerably larger than the average energy content of the grain. This non-equilibrium grain heating can change significantly the energy distribution of the radiation field in infrared sources. By formulating the radiation transport problem involving transient heating in a fashion similar to a non-LTE line transfer problem involving many transitions, Lis & Leung (1991a,b) recently constructed models which treat self-consistently the thermal coupling between the transient heating of small grains and the equilibrium heating of conventional large grains. They used the models to interpret the IRAS observations of the Barnard 5 cloud and a diffuse cloud in Chamaeleon. In both cases, longward of $100\ \mu\text{m}$, the emission is dominated by large grains. Between $30\text{--}100\ \mu\text{m}$, the emission is produced mainly by very small grains. Shortward of $30\ \mu\text{m}$, both PAHs and small grains are responsible for the emission. Typically very small grains and PAHs account for 10-20% of the total opacity in the visible, and 5-20% of the total dust mass of the cloud. Furthermore, to produce the observed infrared limb brightening, the spatial distribution of small grains and PAHs must be more extended than that of large grains. This has important significance in understanding the origin of small grains and PAHs. Thus detailed radiation transport models now exist which incorporate both the transient heating of very small grains and the equilibrium heating of conventional large grains.

Another important progress deals with the study of grain formation in stellar outflows, using a master-equation approach (Egan and Leung, this volume). This method allows a self-consistent treatment of grain nucleation and growth. It is found that, compared to the classical nucleation theory, the new method predicts fewer but larger grains. This has important observational implications.

2.3 Source Geometry

Although there is growing observational and theoretical evidence for a large number of disk-shaped or toroidal objects of astrophysical interest (e.g., circumstellar disks, protoplanetary disks, protostellar accretion disks, bipolar molecular flows, and disk galaxies), most models currently in use invoke the assumption of spherical geometry. A few attempts have been made to model infrared sources with nonspherical geometry. Lefevre et al. (1983) performed Monte Carlo simulations of ellipsoidal dust shells around cool stars, while Ghosh & Tandon (1985) calculated dust temperature distributions in cylindrical clouds with embedded stars. The latter work has been extended by Dent (1988) to the case of circumstellar disks around young stars. Most recently, Spagna et al. (1991) considered radiation transport in disk-shaped interstellar clouds heated externally by the ambient interstellar radiation field. While theoretical tools are available for modeling infrared sources with different geometries, the typical thousand-fold increase in computing requirement for 2-D geometries makes it impractical to do any extensive modeling. In Figure 3 we compare the two geometries (1-D sphere vs. 2-D disk) from theoretical and observational considerations. Since establishing source geometry places severe constraints on the origin, dynamics, and properties of infrared sources, it is crucial to consider realistic geometries.

either a C-rich or an O-rich remnant shell can. Thus by modeling a class of sources and comparing the results with observations, one can identify trends and determine more reliably the physical source parameters.

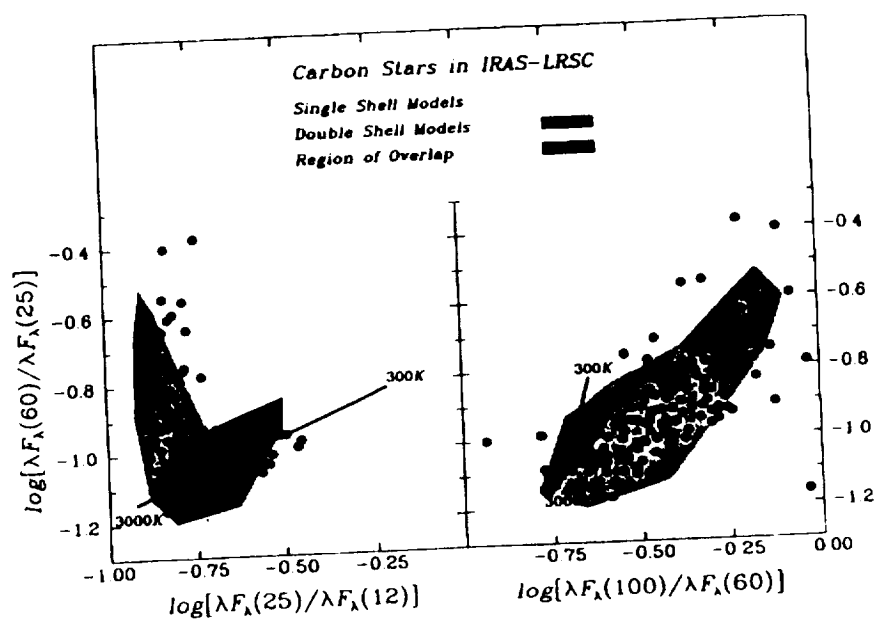


Figure 4 - Color-color diagrams for selected carbon stars in the IRAS data (filled circles). The shaded areas indicate regions occupied by models.

3. CONCLUDING REMARKS AND OUTLOOK

To summarize, much progress has been made in the development of phenomenological models for infrared sources. Models with increasing degree of physical realism have become available. Future research in this area should incorporate other important physical processes so that self-consistent physical models can ultimately be constructed: a) transfer of polarized radiation, b) radiation hydrodynamics, c) radiation transport in 3-D geometries, d) grain nucleation and growth, and e) gas-phase and grain-surface chemistry. In addition, improvements in computational techniques, e.g., better algorithms and iteration procedure, should be made.

Another critical research area deals with automation of modeling. Constructing computer models for specific infrared sources (model fitting) is a labor-intensive task, since one needs to adjust many model parameters and run many models. It is not unusual to require several hundreds of models before one finds a few models which can fit the observations. To expedite the analysis of spaced-based infrared observations, a critical task is to automate the modeling process so that researchers

can model infrared sources on workstations in real time. When computer modeling becomes as easy as doing least-square fits, it will become a routine part of data analysis. With automation researchers can perform computer experiments to test various hypotheses and determine the physical parameters for infrared sources. With such a research tool, predictions on certain observational consequences can be made readily. This will stimulate further observations and theoretical studies, efforts which are essential to the future space-based missions such as ISO and SIRTf.

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